FINAL SYNOPSIS OF THE THESIS ENTITLED

‘STUDY OF OXIDATIONS OF ORGANIC COMPOUNDS- A KINETIC APPROACH’

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DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY
AURANGABAD.

By

RAJESH BHAURAO FADAT

For
Ph.D. Degree in Chemistry

Under the guidance

of
Dr. D.M. Janrao
Associate Professor
Dept. of Chemistry
JES College, Jalna.
(M.S.) 431203.

KINETICS OF OXIDATION OF SOME ORGANIC COMPOUNDS.

Any chemical reaction with its mechanism can be elucidated with the chemical kinetics.

A branch of physical chemistry which deals with the study of rate of reaction and the various factors which can hamper the yield of the overall reaction is termed as chemical kinetics. Kinetics provides an account to understand the optimum conditions which can enhance maximum yield of the reaction:

A chemical reaction mechanism can understand with kinetics:

A chemical reaction involves the breaking of exiting bond which is present in the reactant and making of new bonds in respective product. Such reactions occur by coming the atoms closer or by the transfer of electrons. Reaction mechanisms focus on the various step through which reaction proceed. Chemical kinetics is very useful to understand the each step of the reaction and also it accounts the following different parameters, -

i) The factors that affect the reaction rate.

ii) Optimum condition which is very essential to obtained the desired product.

iii) The intermediate formed during the course of reaction.

iv) At what extent of time the reaction proceeds.

Thus the mechanism of reaction can be easily understood with the help of chemical kinetics. The different factors which affects the rate of reaction such as concentration of reactant, nature of solvent, temperature, catalyst, orientation of reacting species, surface area, ionic strength, intensity of light etc. A probable mechanism of reaction can be elucidated by using the information which obtained by studying the rate of reaction.

Effect of concentration of reactants on the rate of reaction:-

At given temperature rate of reaction is directly proportional to the concentration of the reactant.

i.e. $r \propto C^n$

Where, c-concentration of reactant

n- order of the reaction

or

$$\mathbf{r = KC^n}$$

Where, K-specific rate

According to collision theory an reaction yield a desired product with only effective collision of reactant molecules as the concentration of reactant increases the collision of reaction molecules increase and so the rate of reaction. A decrease in concentration will decrease the rate of reaction.

Nature of reactants:-

As the reaction involves the braking and making of new bonds between reactant and product thus the nature of such bonds can alter the rate of reactions. Generally ionic compounds has tendency to undergo change rapidly than covalent compounds as ionic compounds in water involve only exchange of ions, which are form easily in aqueous solution as ionic compounds dissociated.

Surface area:-

If more surface area of solid reactant is available it will increase rate of reaction. More surface area of reactant can be obtained by crushing it into powder form. Due to more surface area reactant comes closer and desired yield of the product can be easily obtained.

Nature of solvent:-

Rate of reaction is also depends on the nature of solvent used during the course of reaction and it also alter the mechanism of such reaction. There are some reaction in which there may establish electrostatic forces between the reacting molecules and the solvent, in such cases the dielectric constant of solvent play an important role to understand the reaction in detail. There are some reaction which involves formation of dipole in order to study such reaction dielectric constant of solvent must be considered.

Ionic strength :

Ionic strength of the reaction medium plays a crucial role in determination of rate of reaction. Presences of the ions in the solution which is measure of electrical intensity can affect the ionic strength of the solution. How added salt can alter the rate of chemical reaction under consideration can be used as way to know the reaction mechanism.

Significance of Thermodynamic Parameters:

The rate of reaction is related with various thermodynamic parameters like Energy of activation (Ea), free energy factor (A), free energy change (ΔG), Entropy change (ΔS), change

in enthalpy (ΔH) and their magnitude gives very helpful information to account the reaction mechanism. The frequency factors (A) is related with frequency of collision according to collision theory, which is used to measure the entropy of activation in the transition state theory.

Entropy is the measure of the randomness of a system and entropy of activation is the entropy change in going from the reactants to the activated complex. Hence its magnitude depends on the nature of reactants and activated complex. The determination of entropy of activation and its utilization in the prediction of reaction mechanism has been explained. Reaction is said to be normal if $\Delta S = 0$ otherwise it is termed as fast of slow according to whether ΔS value is positive or negative.

Objective of the present work:

For various organic substrate potassium hexacynoferrate (PHCF) in basic medium has been extensively used as oxidizing agent. PHCF as an oxidant plays an important role in various ferrate synthesis and can be used as oxidant in basic and neutral media. To evaluate the oxidizing power of PHCF it was decided to study the kinetic of some organic compounds.

By using spectrophotometric method and under pseudo first order kinetic investigation of oxidation of some organic compounds has been carried out.

In the present study kinetics of oxidation of Oxacillin, Ribavirin, Neomycin, Theophyline and Amoxicillin in aqueous basic medium by sodium hydroxide have been studied. To elucidated reaction mechanism the work involves the determination of,

1) Variation of base, ionic strength, variation of salts, reaction product and variation of oxidants

2) Order with respect to each reactant.

3) Effect of temperature on reaction rate.

Methodologies:

Spectrophotometric method has been employed to investigate the kinetics of oxidation of organic compounds by PHCF in basic media i.e. aqueous sodium hydroxide**.** The product so obtained was analyzed and confirmed by using sophisticated well known techniques like HPLC, TLC and qualitative analysis.

Experimental Details:

All kinetic runs were carried under pseudo first order conditions i.e. with excess of the organic compound over the oxidant at room temperature. An essential amount of substrate, NaOH and water (to maintain a constant volume) were measured and thermally equilibrated for each run.

With stirring the oxidant PHCF is rapidly added to the reaction mixture. A double beam UV-Visible spectrophotometer (Elico-198) was used to monitor the progress of the reaction which has its absorption maximum of 420 nm was as a function of time. The reaction was monitored for 120 seconds. By using the so obtained experimental data pseudo –first order rate constant K was calculated. The effect of salts like $NaHCO_3$, NaCl, Na_2CO_3, NH_4Cl, NH_4Br, KCl, KBr, KI, KNO_3, and K_2SO_4, were studied.

***Stiochiometry*:** The unconsumed oxidant i.e. PHCF was determined spectrophotometrically for reactions which was kept for 24 hours with various set of concentration of reactants. The product of the reaction so obtained was isolated and analyzed.

PRESENT WORK

The thesis entitled, "Study of Kinetics of Organic Compounds-A Kinetic Approach", explain the detailed reaction mechanism of ferrate oxidation of Oxicillin, Ribavirin, Neomycin, Theophyline and Amoxicillin using a double beam UV-Visible spectrophotometer (Elico-198) under basic condition.

The thesis is divided into four chapters

Chapter 1 INTRODUCTION

This chapter covers the general chemistry of various oxidation reactions, their kinetics and mechanisms using PHCF as an oxidizing agent. A survey of literature has been made to account for the ferrate oxidation of some organic compounds in basic media. Scope of the present work has been reported at end of this chapter.

Chapter 2 EXPERIMENTAL

The second chapter elaborates the experimental details, consisting of method employed to purify the chemicals, a short account of the apparatus and instruments used for the study of kinetics, known methods for preparation and estimation of reagents. For the determination of stoichiometry and product analysis known methods employed. To follow the reaction, to determine the rate constant and thermodynamic parameters known methods are used and deal in detail.

Chapter 3

This Chapter includes experimental Results and is divided into five sections.

Section: A Kinetics of Ferrate oxidation of Oxacillin in basic media.

This section presents the studies concerning the kinetics of ferrate oxidation of oxacillin in basic media.

Section: B Kinetics of Ferrate oxidation of Ribavirin in basic media.

This section includes the kinetics of ferrate oxidation of ribanirin in basic media.

Section: C Kinetics of Ferrate oxidation of Neomycin in basic media.

This section presents the studies concerning the kinetics of ferrate oxidation of neomycine in basic media.

Section: D Kinetics of Ferrate oxidation of Theophyline in basic media.

This section presents the studies concerning the kinetics of ferrate oxidation of theophyline in basic media.

Section: E Kinetics of Ferrate oxidation of Amoxicillin in basic media.

This section presents the studies concerning the kinetics of ferrate oxidation of amoxicillin in basic media.

In above five sections the tables and graphs representing the results of variation and its effects on following parameters on reaction rate are studied,

I) Oxidant

II) Substrate

III) OH^- (base)

IV) Ionic Strength

V) Temperature.

VI) Reaction product

Chapter 4 Discussion

It describes the results found in earlier chapter and how they are correlated with work of various research analyst. In order to determine the reaction mechanism various mechanistic criteria was reviewed and employed. Based on it suitable mechanism is suggested related with the experimental facts. Finally using mechanistic model the rate law has been derived.

ORIGINAL WORK

Oxidation of some organic compounds by using PHCF in basic media was investigated by spectrophotometrically. A Kinetic mechanistic approach has been made for investigations of oxidation of various compounds by PHCF were reported first time. Thermodynamic parameters and rate determining step were evaluated. Thus, the method so adopted has wide applications for determining the rate law and mechanism of different types of chemical reactions.

Rajesh B. Fadat
Research Student

Dr. D.M. Janrao
Research Guide